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Prediction of Gas Sensing Materials Using Machine Learning Algorithms

There is a growing need for safer homes, environments, and industries; this can be achieved by having gas sensors that are more efficient, cost-effective, and have low power consumption. However, currently used materials for gas sensing have limitations, calling for a need to search for materials with optimal and desired gas-sensing properties. Traditional methods, such as density functional theory, have been used extensively to explore and predict gas-sensing material properties such as adsorption energy, band gaps and response time. Traditional approaches often impede the search for materials' properties because they are time-consuming and computationally costly. This study uses the machine learning approach to predict the properties of gas-sensing materials. The performance of different machine learning algorithms, namely, support vector machine, random forest regressor, gradient boosting regressor, and extra gradient boosting regressor, is evaluated, our results shows that the extra gradient boosting regressor scored R2 of ~ 89%, followed by the gradient boosting regressor, recording a score of 85%; both algorithms had low root mean square errors of 0.70 and 0,95, respectively. This study demonstrates the robustness of ML algorithms to learn and study the pattern of gas-sensing materials for the adsorption of various toxic gases on different surface materials based on the DFT calculated and experimental results for selected descriptors for feature engineering.By training the ML models with the dataset, it can be concluded that prediction with ML is fast and cost-effective, with the ML models' accuracy evaluated using the metrics evaluation of root mean square error (RMSE) and coefficient of determination (R2).

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